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Properties of the semiclassical functionals in the case of broken time reversal symmetry

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Abstract. Starting with a general one-body Hamiltonian which includes an $\vec{\alpha} \cdot \vec{p}$ term describing the coupling between orbital motion and the arbitrary vector field $\vec{\alpha}$, we investigate some properties of the semiclassical functionals of various physical quantities. In particular, we show that these functionals could be written in a very compact way. An approximate expression for the non-interacting total kinetic energy is given. We also show that these approximate semiclassical functionals transform by gauge transformation exactly as the corresponding exact quantum functionals.

1. Introduction

Density functional theory is of considerable interest in the study of the properties of quantum many-body systems. Following the theorem of Hohenberg and Kohn [1], the ground-state energy of a many-body system (including kinetic, exchange and correlation energies) can be represented as a universal functional of the density $n(\vec{r})$. The theorem merely guarantees the existence of such a functional, but unfortunately the exact form of the latter is not known. At this level one can perform a density variational calculation in the strict sense, i.e. the local density is the direct variational quantity. In contrast to this scheme, the Kohn–Sham method [2] uses the single-particle wavefunction $\varphi_j(\vec{r})$ as the basic variable and then treats the kinetic energy part exactly. However, in the density variational calculation, one needs to know an approximate form of the kinetic and the exchange–correlation energy functionals. For the kinetic energy part this is done automatically through the use of a semiclassical approximation. At the lowest order, this is the well known Thomas–Fermi (TF) theory. Its extension is called the extended Thomas–Fermi (ETF) method, in which an expansion of the kinetic energy functional is derived in terms of gradients and higher derivatives of the local density. This is achieved by an expansion of the density matrix in powers of \hbar [3].

In the present paper, we are interested in an approximate semiclassical functional of the non-interacting total kinetic energy part T_S , making use of the ETF method. The time reversal symmetry is broken by the presence of the $\vec{\alpha} \cdot \vec{p}$ term in the Hamiltonian. In this situation, finite orbital current and polarization spin density appear in the ground state. We also investigate the properties of the semiclassical current and spin densities generated by the field $\vec{\alpha}$.

The paper is organized as follows. In section 2 we show that the semiclassical functionals derived up to \hbar^2 terms by Grammaticos and Voros [4] for the various densities given below can be written in a very simple form. A compact form for the total non-interacting kinetic energy density is obtained. In section 3 we show that these semiclassical (ETF) densities satisfy the same gauge transformation laws as the corresponding exact quantum densities defined in

terms of the individual wavefunctions $\varphi_j(\vec{r})$. Section 4 is devoted to the extension of the above property with the inclusion of the spin degrees of freedom. As a particular case, the orbital motion in a magnetic field is briefly treated in section 5. We summarize our results in section 6 and suggest a possible extension of this work.

2. Semiclassical functionals for spin independent Hamiltonian

Consider the general one-body Hamiltonian

$$H_0 = -\frac{\hbar^2}{2m} \vec{\nabla} \cdot f(\vec{r}) \vec{\nabla} + \frac{\hbar}{2i} (\vec{\nabla} \cdot \vec{\alpha}(\vec{r}) + \vec{\alpha}(\vec{r}) \cdot \vec{\nabla}) + V + \frac{1}{2} m \frac{(\vec{\alpha})^2}{f} \quad (2.1)$$

where V and $\vec{\alpha}$ are position-dependent scalar and arbitrary vector fields, respectively.

Let $m^*(\vec{r})$ denote the effective mass value of the particle, which differs from the free mass m . The form factor f is defined as

$$f(\vec{r}) = \frac{m}{m^*(\vec{r})}. \quad (2.2)$$

We assume f to be a position-dependent function to allow the study of more general situations. The one-body wavefunction $\varphi_j(\vec{r})$ satisfies the following eigenvalue equation

$$H_0 \varphi_j = \varepsilon_j \cdot \varphi_j \quad (2.3)$$

with ε_j being the corresponding energy.

Recall that the quantum non-interacting density (number density) $n(\vec{r})$ and the probability current density (paramagnetic current) $\vec{j}_P(\vec{r})$ are respectively defined in terms of φ_j as

$$n(\vec{r}) = \sum_{j=1}^N \varphi_j^* \cdot \varphi_j \quad (2.4)$$

$$\vec{j}_P(\vec{r}) = \frac{\hbar}{2mi} f \sum_{j=1}^N [\varphi_j^*(\vec{r}) \cdot \vec{\nabla} \varphi_j(\vec{r}) - \varphi_j(\vec{r}) \cdot \vec{\nabla} \varphi_j^*] \quad (2.5)$$

where N is the total number of particles.

The total non-interacting kinetic energy of the N particles system with effective mass m^* is given by

$$T_S = \int \tau(\vec{r}) d^3r \quad (2.6)$$

with $\tau(\vec{r})$ being the local kinetic energy defined as

$$\tau(\vec{r}) = \frac{\hbar^2}{2m} f \sum_{j=1}^N [\vec{\nabla} \varphi_j^* \cdot \vec{\nabla} \varphi_j]. \quad (2.7)$$

One notes the presence of the f factor in the \vec{j}_P and τ densities due to the effective mass of the particle.

For the Hamiltonian given by (2.1), Grammaticos and Voros [4] have given functional relations for $\vec{j}_P(\vec{r})$ and $\tau(\vec{r})$ densities in terms of the local density $n(\vec{r})$ and the field $\vec{\alpha}(\vec{r})$, up to \hbar^2 terms. Their Hamiltonian does not include the $\frac{1}{2} m (\vec{\alpha})^2 / f$ term; we add it here in order to work with a gauge invariant theory. These functionals have been used in the context of nuclear physics for the investigation of nuclear rotation [5]. We report here their results, which are

$$\vec{j}_P^{\text{scl}}(\vec{r}) = -n(\vec{r}) \cdot \vec{\alpha}(\vec{r}) + (\delta \vec{j}) \quad (2.8)$$

where the superscript scl emphasizes the semiclassical character of these quantities. In (2.8) the first term on the right-hand side is the usual TF current and $(\delta \vec{j})$ is an \hbar^2 correction beyond the TF method, given by

$$(\delta \vec{j}) = (3\pi^2)^{-2/3} \frac{n^{1/3}(\vec{r})}{4} \left\{ \vec{\nabla}(\vec{\nabla} \cdot \vec{\alpha}) - \vec{\nabla}^2 \vec{\alpha} + \frac{1}{f} [(\vec{\nabla}^2 f + \vec{\nabla} f \cdot \vec{\nabla}) \vec{\alpha} - (\vec{\nabla} \cdot \vec{\alpha} + \vec{\alpha} \cdot \vec{\nabla}) \vec{\nabla} f] \right. \\ \left. + \frac{1}{f^2} [\vec{\nabla} f \times (\vec{\nabla} f \times \vec{\alpha})] + \frac{1}{3n} \vec{\nabla} n \times \left[(\vec{\nabla} \times \vec{\alpha}) - \frac{1}{f} (\vec{\nabla} f \times \vec{\alpha}) \right] \right\}. \quad (2.9)$$

Using the same notation as in (2.8), the kinetic energy density is given by

$$\tau^{\text{scl}}(\vec{r}) = \tau_0(\vec{r}) + \frac{1}{2} m n(\vec{r}) \frac{(\vec{\alpha})^2}{f} + (\delta \tau) \quad (2.10)$$

with τ_0 being the usual ETF functional in the case $\vec{\alpha} = 0$ [3]. This term depends only upon the density $n(\vec{r})$ and its derivatives. The second term is the TF collective energy due to the field $\vec{\alpha}$. The second-order contributions of the field $\vec{\alpha}$ to $\tau^{\text{scl}}(\vec{r})$ are given by

$$(\delta \tau) = \frac{1}{2} m (3\pi^2)^{-2/3} \frac{n^{1/3}(\vec{r})}{f} \left\{ \frac{1}{4} \vec{\alpha} \cdot \vec{\nabla}^2 \vec{\alpha} + \frac{1}{8} \vec{\nabla}^2 (\vec{\alpha})^2 - \frac{1}{4} \vec{\nabla}(\vec{\alpha} \cdot \vec{\nabla}) \vec{\alpha} - \frac{1}{2} (\vec{\alpha} \cdot \vec{\nabla})(\vec{\nabla} \cdot \vec{\alpha}) + \frac{1}{2f} \right. \\ \times [-2\vec{\alpha} \cdot (\vec{\nabla} f \cdot \vec{\nabla}) \vec{\alpha} - (\vec{\alpha})^2 \cdot \vec{\nabla}^2 f + (\vec{\alpha} \cdot \vec{\nabla})^2 f + (\vec{\alpha} \cdot \vec{\nabla} f)(\vec{\nabla} \cdot \vec{\alpha}) + \vec{\nabla} f (\vec{\alpha} \cdot \vec{\nabla}) \vec{\alpha}] \\ \left. + \frac{3}{4f^2} (\vec{\alpha} \times \vec{\nabla} f)^2 + \frac{1}{6n} (\vec{\nabla} n \times \vec{\alpha}) \left[(\vec{\nabla} \times \vec{\alpha}) - \frac{1}{f} (\vec{\nabla} f \times \vec{\alpha}) \right] \right\}. \quad (2.11)$$

Denote by \vec{v} the quantity $\vec{\alpha}/f$ and substitute it in the expressions $(\delta \vec{j})$ and $(\delta \tau)$ already given above. A considerable simplification occurs and the final result can be written in a very compact way as

$$(\delta \vec{j}) = (3\pi^2)^{-2/3} \frac{1}{4} (\vec{\nabla} \times \vec{G}) \quad (2.12)$$

$$(\delta \tau) = \frac{1}{2} m (3\pi^2)^{-2/3} \left[\frac{1}{2} \vec{\nabla} \cdot \left(\frac{\vec{\alpha}}{f} \times \vec{G} \right) - \frac{f n^{1/3}}{4} \left(\vec{\nabla} \times \frac{\vec{\alpha}}{f} \right)^2 \right] \quad (2.13)$$

with \vec{G} being the following vector:

$$\vec{G} = f n^{1/3} \left(\vec{\nabla} \times \frac{\vec{\alpha}}{f} \right). \quad (2.14)$$

When integrated over the whole space, the first term in (2.13) vanishes. This allows us to give the following compact expression for T_s using (2.6) and (2.10) up to order \hbar^2

$$T_s = \int \tau_0(\vec{r}) d^3r + \frac{1}{2} m \int n(\vec{r}) \cdot \frac{(\vec{\alpha})^2}{f} d^3r - \frac{1}{8} m (3\pi^2)^{-2/3} \int f n^{1/3} \left(\vec{\nabla} \times \frac{\vec{\alpha}}{f} \right)^2 d^3r \quad (2.15)$$

where we recall that the first real term is obtained for vanishing field $\vec{\alpha}$, and is explicitly given in [3].

3. Local gauge transformation of semiclassical densities

Let us now recall the gauge transformation rules of the exact quantum densities given respectively by (2.4), (2.5) and (2.7). Under a local gauge transformation of the Slater determinant $|\Psi\rangle$, constructed out of the φ_j 's, one can write

$$|\Psi'\rangle = \exp \left[i \sum_{j=1}^N \Phi(\vec{r}_j) \right] |\Psi\rangle \quad (3.1)$$

where $\Phi(\vec{r}_j)$ is an arbitrary scalar function.

In this gauge transformation each individual function φ_j is multiplied by a phase factor $\exp(i\Phi(\vec{r}_j))$. By imposing the f factor to be gauge invariant, the gauge transformed densities are

$$n(\vec{r}) \rightarrow n'(\vec{r}) = n(\vec{r}) \quad (3.2)$$

$$\vec{j}_P(\vec{r}) \rightarrow \vec{j}'_P(\vec{r}) = \vec{j}_P(\vec{r}) + \frac{\hbar}{m} f n(\vec{r}) \cdot \vec{\nabla} \Phi \quad (3.3)$$

$$\tau(\vec{r}) \rightarrow \tau'(\vec{r}) = \tau(\vec{r}) + \hbar \vec{j}_P(\vec{r}) \cdot \vec{\nabla} \Phi + \frac{\hbar^2}{2m} f n(\vec{\nabla} \Phi)^2. \quad (3.4)$$

These transformation laws are strong constraints. To be admissible, any approximate form of these densities is bound to satisfy these transformation laws. Before going to the semiclassical functionals, we mention that the transformed wavefunction $\varphi'_j = \exp(i\Phi)\varphi_j$ is a solution of the same Schrödinger equation as φ_j , provided we make the following generalized substitution

$$\vec{\alpha} \rightarrow \vec{\alpha} - \frac{\hbar m}{f} \vec{\nabla} \Phi. \quad (3.5)$$

Consider now the gauge transformation of the field $\vec{\alpha}$, given by (3.5). The vector \vec{G} , (2.14) and consequently (δj) , (2.12), are gauge invariant. Then one can easily verify that the full semiclassical paramagnetic current \vec{j}_P^{scl} transforms exactly as the corresponding quantum paramagnetic current, equation (3.3).

Let us now calculate the gauge transformed, semiclassical, kinetic energy density denoted by $\tau^{\text{scl}'}$ (see equations (2.10) and (2.13)). The latter contains three terms. The τ_0 term, which depends only upon $n(\vec{r})$ density, is gauge invariant

$$\begin{aligned} \tau^{\text{scl}'} = \tau_0 + \frac{1}{2} m n f \left(\frac{\vec{\alpha}}{f} - \frac{\hbar}{m} \vec{\nabla} \Phi \right)^2 + \frac{1}{2} m (3\pi^2)^{-2/3} \\ \times \left\{ \frac{1}{2} \vec{\nabla} \cdot \left(\left(\frac{\vec{\alpha}}{f} - \frac{\hbar}{m} \vec{\nabla} \Phi \right) \times \vec{G} \right) - \frac{f n^{1/3}}{4} \left(\vec{\nabla} \times \frac{\vec{\alpha}}{f} \right)^2 \right\} \end{aligned} \quad (3.6)$$

so one obtains

$$\tau^{\text{scl}'} = \tau^{\text{scl}} + \frac{\hbar^2}{2m} n f (\vec{\nabla} \Phi)^2 - \hbar n \vec{\alpha} \cdot \vec{\nabla} \Phi - \frac{\hbar}{4} (3\pi^2)^{-2/3} \vec{\nabla} \cdot [\vec{\nabla} \Phi \times \vec{G}]. \quad (3.7)$$

To evaluate the last term we use the following relation for any two vectors \vec{A} and \vec{B} ,

$$\vec{\nabla} \cdot (\vec{A} \times \vec{B}) = \vec{B} \cdot (\vec{\nabla} \times \vec{A}) - \vec{A} \cdot (\vec{\nabla} \times \vec{B}) \quad (3.8)$$

and by using the expression of j_P^{scl} density, (2.8) and (2.12), one finally gets

$$\tau^{\text{scl}'} = \tau^{\text{scl}} + \frac{\hbar^2}{2m} n f (\vec{\nabla} \Phi)^2 + \hbar \vec{j}_P^{\text{scl}} \cdot \vec{\nabla} \Phi \quad (3.9)$$

which is the desired result.

Finally we note that, from the n , \vec{j}_P and τ densities, one can build two local gauge invariant quantities. The first one is the vorticity $\vec{c} = \vec{\nabla} \times (\vec{j}_P/n)$ and the second is the scalar $\tau - (m/2f)(\vec{j}_P^2/n)$. The latter represents the local non-collective kinetic energy. From the above analysis the corresponding semiclassical quantities are also local gauge invariants.

4. Spin-dependent Hamiltonian case

Let us now extend the one-body Hamiltonian by adding the term $\hbar \vec{B}_0 \cdot \vec{\sigma}$:

$$H = H_0 + \hbar \vec{B}_0 \cdot \vec{\sigma}. \quad (4.1)$$

The field \vec{B}_0 is supposed to be gauge invariant. It may contain many contributions, such as the coupling of the external field with the spin, exchange-correlation and spin-orbit coupling. We limit ourselves to a simple case of the first type of coupling and recall that for spin $\frac{1}{2}$ the vector $\vec{\sigma}$ has as components the usual 2×2 Pauli matrices.

Any operator of interest can be expressed as a 2×2 matrix of operators. In particular, the density matrix operator is defined by

$$\hat{n} = \frac{1}{2}(\hat{n}_0 + \vec{n} \cdot \vec{\sigma}). \tag{4.2}$$

We are only interested in local quantities, therefore in spatial coordinates one has

$$n_0(\vec{r}) = \sum_{\sigma} \langle \vec{r}, \sigma | \hat{n} | \vec{r}, \sigma \rangle \tag{4.3}$$

$$\vec{n}(\vec{r}) = \sum_{\sigma} \langle \vec{r}, \sigma | \hat{n} \cdot \vec{\sigma} | \vec{r}, \sigma \rangle \tag{4.4}$$

with $n_0(\vec{r})$ and $\vec{n}(\vec{r})$ being respectively the scalar and the vector spin densities.

In [6] Grammaticos and Voros extended their work to spin-dependent Hamiltonians. For the simplified Hamiltonian, (4.1), the \vec{j}_p^{sc1} and τ^{sc1} densities remain unchanged, and they obtain the following functional for the spin density

$$\vec{n}(\vec{r}) = -\frac{3m(3\pi^2)^{-2/3}}{\hbar f} n_0^{1/3} \vec{B}_0 \tag{4.5}$$

which is local gauge invariant.

5. Application to a particular case: orbital motion in a magnetic field

In our approach the constraining field $\vec{\alpha}$ may result from several external fields $\vec{\alpha} = \sum_i \vec{\alpha}_i$. It can also incorporate an exchange-correlation contribution in a self-consistent approach. In this section we treat a simple example of only one external vector field. Suppose an electron system in a three-dimensional $V(\vec{r})$ scalar potential is subjected to a magnetic field \vec{B} . The one-body Hamiltonian in the case of constant effective m^* mass (ignoring the spin degrees of freedom) is given by

$$H = \frac{1}{2m^*} \left(\frac{\hbar}{i} \vec{\nabla} + \frac{e}{c} \vec{A} \right)^2 + V(\vec{r})$$

where \vec{A} is the vector potential related to \vec{B} by $\vec{B} = \vec{\nabla} \times \vec{A}$ (note $e > 0$). It can be easily seen that the above Hamiltonian is a particular case of the one given by (2.1) by just putting $\vec{\alpha} = (e/m^*c)\vec{A}$. Let us report here the expression of the total kinetic energy

$$T_S = \int \tau_0(\vec{r}) d^3r + \frac{e^2}{2m^*c^2} \int n(\vec{r}) \cdot \vec{A}^2 d^3r - \frac{e^2}{8m^*c^2} (3\pi^2)^{-2/3} \int n^{1/3} \vec{B}^2 d^3r.$$

This expression is useful in a variational-type calculation. The corresponding expressions for the \vec{j}_p^{sc1} and τ^{sc1} densities are obtained in a similar way by using, respectively, (2.8), (2.10) and (2.12), (2.13).

A more complete analysis will be presented in a forthcoming work, which will also include the contribution of the spin degrees of freedom. A direct link will be made between these semiclassical functionals and the work of Vignale *et al* [7] on the current-density functional theory.

6. Conclusion

Using the semiclassical ETF approach, for a general spin-dependent one-body Hamiltonian, we have shown that the various ETF densities could be written in a greatly simplified way. We have obtained a compact expression for the total kinetic energy. We have also shown that the semiclassical ETF functionals obey the gauge transformation laws as the exact quantum functionals. Grammaticos and Voros [4] obtained the various functionals up to \hbar^4 terms in the case of $\vec{\alpha} = 0$ and up to \hbar^2 terms only in the case of a non-vanishing field $\vec{\alpha}$. This is due to the lengthy expressions in the latter case. From the present analysis, we can conclude that these fourth-order terms, which have not been calculated, must be gauge invariant in order to satisfy the exact gauge transformation laws. Finite-temperature ETF functionals have also been derived in the absence of the vector field [8]. We extend these calculations to the present functionals of a non-vanishing field case. Our results will be presented in a forthcoming work.

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